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Internal Conversion Coefficients – How good are they now?

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Abstract. The internal conversion and electron–positron pair creation processes provide a versatile tool for investigating various aspects of the nuclear structure. The most recent calculations of Internal Conversion Coefficients (ICC), are based on relativistic self–consistent Dirac-Fock calculations and are widely regarded as the most accurate numerical results available today. However one of the remaining challenges for both theory and experiment is the treatment of the atomic shell vacancy created in the conversion process. The last review of the field by Raman *et al.* [1] in 2002 concluded, that the effect of the hole could be excluded from the calculations. The new experimental K conversion coefficient of the 80.2 keV M4 transition in ^{193}Ir [2], published recently, indicate that the effect should be included. In this paper we report on an extended review of experimental conversion coefficients, which are compared to two extreme assumptions on the effect of the vacancy. Based on our results, the international network of Nuclear Structure and Decay Data (NSDD) evaluators has adopted a new theoretical conversion coefficient table based on the so–called "Frozen Orbitals" approximation. We also report on the development of a new comprehensive conversion data base which has been adopted for the NSDD network.

INTRODUCTION

Since the first observation of monoenergetic electrons in radioactive decay by O. Hahn and L. Meitner [3] in 1924, the study and the use of the internal conversion process has been central to experimental nuclear structure research. An electromagnetic decay of the atomic nucleus can proceed by the emission of

(a) a photon (γ),
(b) an orbital electron (e^-, internal conversion, CE),
(c) an electron–positron pair (internal pair formation, IPF)
(d) two photons, *etc.* (higher order processes with relative probability less than $\sim 10^{-3}$ to $\sim 10^{-4}$).

The so–called conversion coefficient, α_{ce} is defined as the ratio of the electron emission rate (T_{ce}) to the gamma emission rate (T_γ), $\alpha_{ce} = T_{ce}/T_\gamma$. Similarly, the conversion coefficient involving electron–positron pair emission rate (T_{IPF}) is defined as $\alpha_{IPF} = T_{IPF}/T_\gamma$. For transitions between spin zero states, $0_i^+ \rightarrow 0_f^+$ or $0_i^- \rightarrow 0_f^-$, the emission of a single γ–photon is strictly forbidden by considerations of angular-momentum conservation and, therefore, a conversion coefficient is not defined for these type of transitions.

The internal conversion and electron–positron pair creation processes have proven to be versatile tools to study nuclear structure. The conversion coefficient depends on the atomic number (Z), the transition energy (E_γ), the transition multipolarity (πL), and in the case of internal (electron) conversion, the atomic shell involved. By comparing measured and calculated conversion coefficients in many cases one can determine transition multipolarities and then infer spin–parity for the excited states involved. However, the question of *"How good the conversion coefficients are now?"* has always challenged both the theoretical calculations and the experiments. The recent survey of the data by Raman *et al.* [1] in 2002 concluded, that there is a systematic discrepancy of $\sim$3% between experiment and the two most widely used theoretical tabulations of Hager and Seltzer [4] and Rösel *et al.* [5, 6]. The former table, augmented with the tabulations of Dragoun *et al.* [7] for the outer shells has been used in the last 25 years for the Evaluated Nuclear Structure Data File (ENSDF) [8, 9], a computer-based file system designed to store nuclear structure information.

Significantly improved calculations have been carried out by Band, Trzhaskovskaya, Nestor, Tikkanen and Ra-

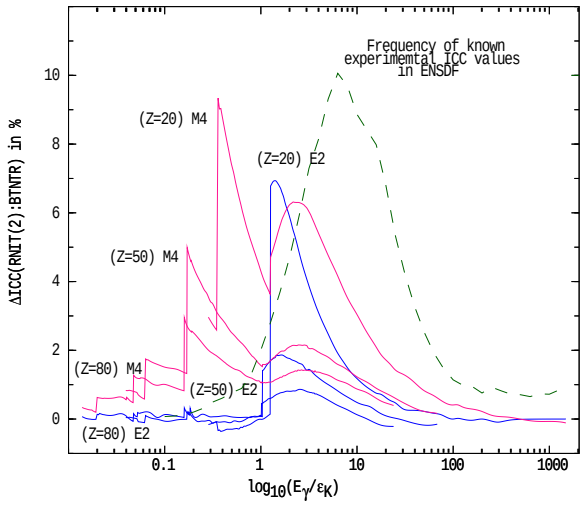

FIGURE 1. Difference (in percentage) between calculated total conversion coefficients using the *'Frozen Orbitals'* (RNIT(2)) and *'No Hole'* (BTNTR) approximations for Z=20, 50 and 80 atomic numbers and E2 and M4 multipolarities as a function of transition energy divided by the K-binding energy. Dashed line indicate the frequency distribution of the known α_{total} values [8].

man [10]. Their calculations are based on the relativistic Dirac-Fock (DF) method in which the exchange interaction between bound electrons as well as between bound electrons and the conversion electrons is included exactly. The new DF model can incorporate the effect of the atomic vacancies in two different ways. While in one approximation it is assumed that the hole is filled instantaneously (*'No Hole'*), in the other case (*'Frozen Orbitals'*) it is assumed that the atomic recombination time is much longer than the time needed for the electron to escape. Using a set of 100 experimental conversion coefficients, measured to better than 5% accuracy, Raman *et al.* [1] carefully compared the experimental values to the various theoretical calculations. Their analysis showed that, on average, the new DF calculations, based on the *'No Hole'* approximation agree with experiment better than 0.5% ($+0.19 \pm 0.26\%$) and they have recommended adopting it for future work. It should be noted, that the average difference between experiment and theory using the *'Frozen Orbitals'* approximation is only marginally larger ($-1.18 \pm 0.24\%$) and there has been a growing concern that the effect of the atomic vacancy should not be ignored.

REVIEW OF THE HIGH PRECISION EXPERIMENTAL CONVERSION COEFFICIENTS

Previous comparisons of experimental and theoretical conversion coefficients have included total and K-shell conversion coefficient of transitions with E2, M3, E3, M4, E4 and E5 multipolarity. It was assumed that this set of data provide the best benchmark test. In comparing $\alpha_{ce}(Exp)$ and $\alpha_{ce}(theor)$ values it should be noted that the difference in theoretical conversion coefficients based on the *'No Hole'* and on the *'Frozen Orbitals'* approximations depends on Z, E_γ, τL and on the electronic shell. This is illustrated on Fig. 1, which shows the difference in α_{total} values for a range of Z values and for E2 and M4 multipolarities. Plotting values as a function of E_γ/ε_K, where ε_K is the K–shell binding energy, allows to visualize some of the common features:

(a) The largest differences are expected just above the K–shell binding energies.

(b) The differences are similar for the various Z-values on the E_γ/ε_K scale.

(c) For E2 transitions there is very little difference below the K-shell binding energy.

(d) M4 multipolarities the $\Delta ICC(RNIT(2) : BTNTR)$ difference is less prominent for outer shells.

Also shown in the figure is the frequency spectrum of the α_{total} values constructed from data given in the ENSDF [8] file. From this figure one can estimate the impact of adopting one or the other approximation on the α_{total} values and hence the total transition intensities.

Our intention was to review and possibly extend the list of experimental conversion coefficient, assembled by Raman *et al.* [1]. It was motivated by the new experimental value of $\alpha_K = 103.0(8)$ of the 80.2 keV M4 transition in ^{193}Ir published by Nica *et al.* [2] in 2004. It is in excellent agreement with the value of $\alpha_K(theor) = 103.3(3)$ calculated using the *'Frozen Orbitals'* approximation. On the other hand the *'No Hole'* approximation gives a value of 92.0(3), which is about 11% lower than the experimental one.

The revised list of high precision experimental conversion coefficients contains about 140 transitions. Our approach was to critically review the original data using up–to–date information on quantities, for example fluorescence yields, and to consider all published measurements. While most of the corrections to the adopted values in the ENSDF file were small, at the $\sim 1-2\%$ level; in a number of cases the experimental values changed as much as $\sim$8%. Unfortunately most of the data points are at high energy, where the differences are expected to be

small. A full account of the review will be given elsewhere [11].

Comparing our result to the previous review of Raman *et al.* [1], possibly the largest change in the average differences was obtained in the case of the K–conversion coefficients. Figure 2 compares 64 α_K values, representing more than 50% of all cases considered, with the theoretical α_K obtained with *'No Hole'* approximation. The average difference deduced is $+1.8(5)\%$, which is significantly larger than the $+0.5(5)\%$ reported earlier [1]. Table 1 summarizes the average differences for the various groups of multipolarities and shells. In the case of the K/L ratio there might be a systematic difference between experiment and theory, as the average difference values are relatively large negative numbers for both approximations. The fact, that the average differences between the experimental and the *'Frozen Orbitals'* (RNIT(2)) approximation are all around -1% and that the similar figures for the *'No Hole'* (BTNTR) approximation display a significant scatter, could be interpreted as a preference toward the former model. There are a few transitions with larger than 5% uncertainties, which have been excluded from the review, but the difference between the corresponding theoretical values is larger than the experimental uncertainty. For example the experimental value for the 13.2845 keV E2 transition in ^{73}Ge, $\alpha_K(exp) = 297(20)$, is in good agreement with the value of $\alpha_K(theor) = 298.7$ based on *'Frozen Orbitals'* approximation. On the other hand the $\alpha_K(theor) = 264.8$ value, obtained with the *'No Hole'* approximation, is 12% lower than experiment, which also supports our recommendation to adopt a the *'Frozen Orbitals'* (RNIT(2)) approximation. This recommnedation was endorsed by the recent meeting of the international network of the Nuclear Structure and Decay Data evaluators, responsible for maintaining the ENSDF data base.

TABLE 1. Average differences (in %) between accurately measured and theoretical internal conversion coefficients.

Multi-polarity[a]	Shell[b]	N	$\overline{\Delta ICC}$ in %	
			(Exp:BTNTR)	(Exp:RNIT(2))
All	All	139	+0.58*(28)*	-1.01*(21)*
All	T	57	+0.34*(28)*	-0.87*(26)*
All	K	64	+1.79*(54)*	-0.73*(67)*
All	L	11	-0.22*(64)*	-0.56*(65)*
All	K/L	5	-2.9*(11)*	-4.9*(11)*
All	T&K	121	+0.87*(29)*	-0.82*(21)*
E2	All	69	-0.26*(39)*	-1.17*(36)*
E2	T	35	-0.10*(42)*	-0.88*(41)*
E2	K	26	+0.74*(62)*	-0.47*(42)*
E3	All	18	+0.9*(12)*	-0.8*(12)*
E3	T	5	-0.5*(29)*	-1.8*(29)*
E3	K	9	+3.9*(15)*	+1.3*(16)*
M3	All	5	+1.0*(28)*	-2.2*(23)*
M4	All	41	+0.90*(44)*	-0.97*(18)*
M4	T	14	+0.51*(22)*	-0.84*(22)*
M4	K	21	+2.2*(10)*	-1.16*(37)*

[a] Multipolarities included: E2, M3, E3, M4, E4 and E5.
[b] Experimental α values for T(total), K–, L–shells, K/L and K/L1 ratios.

BRICC – A NEW TOOL TO OBTAIN CONVERSION COEFFICIENTS AND ELECTRONIC FACTORS

Recognizing the continuing need to obtain theoretical conversion coefficients for a wide range of fields, including basic nuclear research, nuclear structure data evaluations, nuclear engineering, applications of radioisotopes, etc. we have developed a new conversion data base and related software. The program Bricc [17] uses cubic spline interpolation to calculate conversion coefficients for a given Z, E_γ, atomic shell and τL multipolarity. The core part of the data base is the Dirac–Fock ICCs for Z=10–95, $1\,keV \leq E_\gamma \leq 6000\,keV$, L=1-5 and for all atomic shells. The calculations are based on the *'Frozen Orbitals'* (RNIT(2)) approximation and were carried out in this study. In regions where the conversion coefficients are changing very sharply, the tabulations use small energy steps in order to improve the numerical accuracy.

The data base also comprises a number of tables for electron–positron pair conversion coefficients [12, 13] and E0 electronic factors, $\Omega(E0)$ [14, 15, 16]. BrIcc can be used interactively to obtain $\alpha_{CE,IPF}$ and $\Omega_{CE,IPF}(E0)$ values or as an ENSDF evaluation tool.

CONCLUSION

We undertook an extensive review of the experimental conversion coefficients known to better than 5% in order to assemble an benchmark data set to test the new Dirac–Fock calculations [10]. The experimental electron conversion coefficients have been compared to theoretical values calculated with the extreme assumptions on the effect of the vacancy created during the conversion process. We found sufficient evidence to conclude that the so–called *'Frozen Orbitals'* approximation, which takes

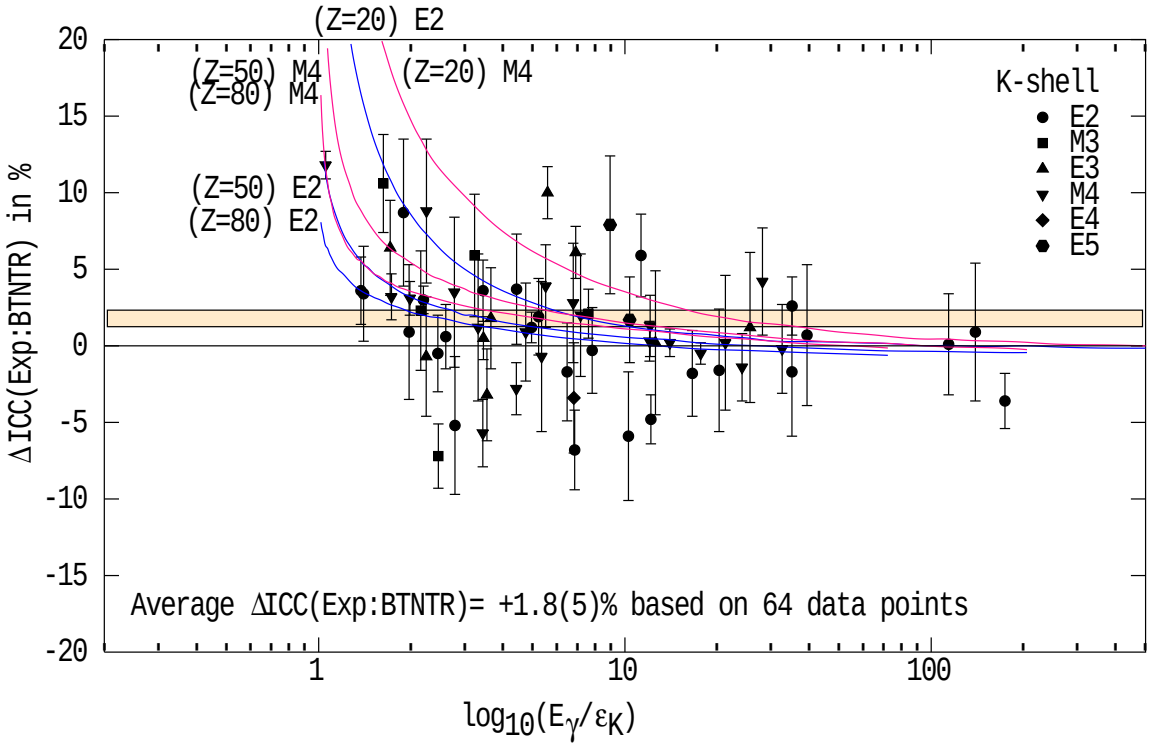

FIGURE 2. Difference (in percentage) between calculated (*'No Hole'* approximation) and experimental K–conversion coefficients. The shaded area represents the average difference of $+1.8(5)$ %. The differences between *'Frozen Orbitals'* (RNIT(2)) and *'No Hole'* (BTNTR) approximations for Z=50 and 80 atomic numbers and E2 and M4 multipolarities are shown as continuous lines. (The horizontal axis is the same as in Fig. 1.)

into account the hole, agrees better with experiment.

A new conversion data base and program has been developed which is now adopted for the international Nuclear Structure and Decay Data network. Further work is planned to extend the new conversion tables for higher Z values and to search for additional experimental evidence to select between the various theoretical models.

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